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NASA Langley Research Center, Hampton, Virginia 23665

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Langley Research Center
Hampton, Virginia 23665



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INTRODUCTION

The Institute for Computer Applications in Science and Engineering (ICASE) is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U. S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis, and computer science in order to extend and improve problem-solving capabilities in science and engineering, particularly in aeronautics and space.

ICASE has a small permanent staff. Research is conducted primarily by visiting scientists from universities and from industry, who have resident appointments for limited periods of time, and by consultants. Members of NASA's research staff also may be residents at ICASE for limited periods.

The major categories of the current ICASE research program are:

- a. Numerical methods, with particular emphasis on the development and analysis of basic numerical algorithms;
- b. Control and parameter identification problems, with emphasis on effective numerical methods;
- c. Computational problems in engineering and the physical sciences, particularly fluid dynamics, acoustics, and structural analysis;
- d. Computer systems and software, especially vector and parallel computers.

ICASE reports are considered to be primarily preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period October 1, 1984, through March 31, 1985, is given in the Reports and Abstracts section which follows a brief description of the research in progress.

Presently, ICASE is operated at NASA Langley Research Center, Hampton, VA under the National Aeronautics and Space Administration, NASA Contracts No. NAS1-17070 and NAS1-17130. In the past, support has been provided by NASA Contracts No. NAS1-15810, NAS1-16394, NAS1-14101, and NAS1-14472.

RESEARCH IN PROGRESS

Loyce M. Adams

Work concerning the convergence questions of parallel (multi-color) SOR was done in conjunction with H. Jordan (University of Colorado). We were able to construct multi-color SOR schemes (for a wide range of stencils used to discretize partial differential equations) with the same rate of convergence as the corresponding natural rowwise ordered SOR scheme. Currently, a grouping of these orderings into equivalence classes for two-dimensional stencils is nearly complete, and an extension to three-dimensional stencils is in progress. The hope is that this classification will aid in choosing an appropriate ordering for SOR to be used with a particular parallel computer architecture.

Work is beginning with M. Patrick (Duke University) to study the effects that different forms of iteration matrices have on communication requirements for parallel computers.

Experience using a different programming environment has been made possible by Caltech. At UCLA, we will shortly be able to use the Caltech simulator for the HYPERCUBE to test ideas by running actual HYPERCUBE programs on the simulator. Once debugged, the algorithms will be run on the actual machine. This work is in conjunction with a graduate seminar I'm teaching on parallel algorithms/architectures. The experience gained should aid the ongoing research at ICASE on parallel algorithms/architectures/programming environments. M. Patrick and I plan to test our algorithms in this manner.

H. Thomas Banks and Kazufumi Ito

We have begun investigations of parameter estimation techniques for second-order hyperbolic systems in variational (or weak) formulation. The problems involve estimation of spatially dependent coefficients (with discontinuities) in systems with elastic and absorbing boundary conditions.

Several types of approximation schemes (Galerkin, tau) in weak variational form are being studied with the use of Legendre polynomials and linear finite elements (splines). Convergence theories for the schemes are similar, but the different types of schemes result in different computational algorithms. These are being investigated theoretically and numerically.

In collaboration with E. Armstrong (LaRC) we are investigating several aspects of feedback control for continuum models. Our basic model is a cantilevered Euler-Bernoulli beam with tip mass and viscoelastic (Kelvin-Voight) damping. Among the topics being pursued are techniques for (1) spectrum analysis; (2) computation of feedback gains (via algebraic Riccati systems as the limit of a system of Chandrasekhar equations) using a Legendre-tau spectral method for approximation; (3) the use of vector and parallel computers in computing feedback controls.

H. Thomas Banks, James M. Crowley, and I. Gary Rosen

We are continuing our efforts on the development of numerical approximation methods for the identification of spatially varying parameters (including stiffness and damping) in hybrid models for the transverse vibration of flexible beams with attached appendages. Our investigations have centered upon a Hilbert space-weak/variational formulation of the coupled system of ordinary and partial differential equations which describes the motion of the system. The approximation schemes are spline-based, both with regard to the infinite dimensional state (using a Galerkin approach) and the infinite dimensional admissible parameter spaces. Current efforts involve investigation of several different optimization schemes in the least-squares based estimation algorithms. Specifically we are comparing quasi-Gauss-Newton methods (Levenberg-Marquardt) with gradients computed via finite differences to quasi-Newton methods such as the BFGS with gradients computed analytically via a costate equation formulation. These efforts are being pursued on conventional sequential computers (Burroughs 6900, IBM 3081) as well as on vector (CRAY 1-S) and array processor (ST-100) architectures exhibiting parallelism.

The efforts on computational work are in collaboration with experimental investigations being conducted by J. Juang (LaRC) and D. Inman (SUNY-Buffalo). Data from their experiments will be used to test our algorithms in the near future.

H. Thomas Banks and K. A. Murphy

We are developing computational techniques for the estimation of temporally, spatially, and state-dependent functional parameters in nonlinear second-order parabolic systems of equations arising in transport models. Both theoretical and numerical investigations are being carried out. We have preliminary findings which suggest that the use of vector architectures can result in practical schemes for the estimation of nonlinearities in problems for which we have not been able to develop feasible schemes on conventional sequential machines.

Alvin Bayliss

The behavior of unstable disturbances in a compressible flow is being simulated numerically. In addition, the control of such disturbances by localized, periodic surface heating and cooling has been simulated. The numerical results have demonstrated that this is a potentially effective technique for flow control in air. The fluctuating disturbances have been followed into a nonlinear regime and the generation of higher harmonics has been observed.

The results have been obtained with a fourth-order accurate finite difference approximation to the Navier-Stokes equations. A three-dimensional version of the code has been developed and is currently being debugged. Extensions of this work to three-dimensional disturbances in transonic and supersonic flows are being planned.

This work is in collaboration with L. Maestrello (LaRC), P. Parikh (Vigyan Associates), and E. Turkel (Tel-Aviv University).

Marsha J. Berger

We have previously studied the accuracy of an adaptive mesh refinement algorithm for solving the Euler equations for steady two-dimensional transonic flow. Using a global coarse grid and locally uniform fine grid patches only where they are needed (such as at the leading and trailing edges and at shocks), the same accuracy can be achieved as a grid that is uniformly refined over the entire domain. A multigrid algorithm has been developed by A. Jameson (Princeton University) to accelerate the convergence to steady state. Work is in progress to extend multigrid to non-global fine grids. The convergence rate appears to depend strongly on how the interface conditions between the fine and coarse grids are handled. We are experimenting with different formulations to try to improve the convergence characteristics.

Shahid H. Bokhari

Research on the problem of augmenting computer networks aims at improving the complexity of an algorithm to reduce the diameter of a graph and also reducing the upper bound on the diameter. This work is in collaboration with A. D. Raza (Telephone & Telegraph Dept., Lahore, Pakistan).

Research on the mapping problem continues in collaboration with M. Ashraf Iqbal (University of Engineering, Lahore, Pakistan). The objectives here are to develop new heuristics and to explore the possibilities of exact solutions for special cases.

The closely related assignment problem for distributed computer systems is also under study. The previously developed dynamic programming solution to the problem of optimally pipelining a chain of tasks over an inhomogeneous unidirectional ring of processors has been extended to the case of two-dimensional meshes.

A multiprocess algorithm for the bin packing problem has been developed and implemented on the HEP (Heterogeneous Element Processor) at Argonne National Laboratories. The performance of this algorithm is being evaluated. An ICASE report is in preparation.

Shahid H. Bokhari and Marsha Berger

The possibilities of solving adaptive mesh refinement problems on a multiprocessor system are being explored. An entirely new method of dissecting the mesh under analysis has been developed. This is based on two-dimensional binary trees and results in an optimal partitioning of the problem. We have analyzed the mapping of such partitionings onto 4-nearest neighbor meshes and onto trees. We are currently analyzing the performance of this technique on hypercubes and shared memory machines. An ICASE report is being prepared.

Dennis W. Brewer

Research is continuing on parameter estimation problems associated with linear evolution equations in infinite-dimensional spaces. A general algorithm based on quasi-linearization has been established along with its local convergence properties. The algorithm has been numerically tested on linear delay-differential equations. Numerical experiments indicate that the method converges rapidly when used to identify two unknown delays together with two or three unknown coefficients using simulated data. Future research will involve continuing numerical experimentation and improvements in the theory to accommodate a wider class of problems.

Dennis W. Brewer, J. Steven Gibson, and I. Gary Rosen

We have developed software for identifying parameters in robotic manipulators. The programs use numerical integration of nonlinear differential equations, nonlinear optimization algorithms, and large matrix computations. This work is in conjunction with J. Pennington and F. Harrison of the LaRC Robotics Group who have provided us experimental data. Parameter values have been obtained for which the model accurately fits the real data over restricted time intervals. Our experience indicates a need to accurately model nonlinear damping dynamics and to develop methods for reducing the parameter sensitivity of the model output. The software needs further development to accommodate noisy data and more complex manipulator dynamics. Also, input optimization for parameters should be a fruitful area for future research. This work should continue through 1985.

Claudio Canuto

A mathematical analysis of some algorithms of spectral type for solving the incompressible Navier-Stokes equations is under way. The aim is to prove rigorous stability and convergence results in terms of the space and time discretization parameters. The Kleiser-Schumann influence matrix method for the Stokes problem has been investigated with G. Sacchi (Istituto di Analisi Numerica del C.N.R.). Other algorithms currently used at LaRC are under consideration.

The Schwarz alternating algorithm is one of the multi-domain algorithms recently proposed for spectral Navier-Stokes calculation in complex geometries (Morchoisne). The convergence properties of this algorithm when applied to elliptic model problems has been studied together with D. Funaro (Istituto di Analisi Numerica del C.N.R.).

Both the previous analyses rely upon the investigation of the behavior of the Chebyshev or Legendre coefficients of the spectral solutions of elliptic boundary layer problems.

Research is continuing with A. Quarteroni (Istituto di Analisi Numerica del C.N.R.) on the efficient use of spectral methods for slow transients simulations in gas ducts.

Stephen F. Davis

Work has continued on the application of upwind finite difference methods to the numerical solution of systems of hyperbolic partial differential equations. Particular emphasis has been focused on methods for computing discontinuous solutions of the Euler equations, i.e., solutions containing shocks.

A recently completed study has shown that it is possible to construct a total variation diminishing (TVD) finite difference scheme which does not require the determination of an "upwind" direction. As a result of this study, a TVD version of the popular MacCormack scheme was constructed and reported on in ICASE Report No. 84-20. At present, a version of this method, applicable to equations written in general non-orthogonal coordinate systems, is being tested by D. Rudy (LaRC). Preliminary results obtained using this scheme compare favorably to results obtained using the more complicated upwind TVD methods.

Currently, this work is proceeding in a number of directions. In particular, we have developed a new limiter for use with the MacCormack TVD scheme and are testing its performance. We are in the process of constructing a central difference TVD artificial viscosity which can be used with implicit schemes, Runge-Kutta schemes, and perhaps spectral methods. We plan to apply these results to both finite volume versions of these algorithms and to equations written in general curvilinear coordinate systems. An ICASE report which describes these developments is in preparation.

A number of researchers have recently noted that diagonally dominant matrices arise from applying Newton-type methods to implicit upwind discretizations of hyperbolic partial differential equations. Since these matrices are amenable to solution by iterative methods, they solve these

problems by applying some iterative method a fixed number (usually one or two) of times per Newton step. Although this approach has been successful, we are currently studying an alternative approach whereby, at each Newton step, the linear system is solved to some tolerance which depends on the size of the Newton residual. Results obtained thus far indicate that this approach requires fewer Newton steps to reach convergence, but at this time we do not know that this yields an overall savings in computational effort for realistic problems.

Work is underway (in collaboration with J. Drummond, LaRC) on numerical methods for problems involving the interaction of fluid dynamics and finite rate chemistry. At present we are conducting a study to determine which of the many methods that have been developed for stiff ordinary differential equations could be practically adapted to large problems involving partial differential equations.

Peter R. Eisman and M. Yousuff Hussaini

The generation and use of solution adaptive grids is assuming an increasing role of importance in the creation of high quality numerical simulation with a limited number of points. This is particularly accented when complex physical processes must be examined and when the point of view is placed upon three-dimensional problems.

In contrast, the use of similarity analysis and more generally the employment of group theoretic methods is appearing to decline in importance as computational capabilities in terms of algorithm and equipment appear to more readily handle cases that otherwise demanded detailed analytical manipulations.

The central feature with this somewhat classical approach was to find the group of transformations which left invariant the given physical equations, to find the corresponding infinitesimal operators, to find the similarity variables, to obtain the simplifying similarity forms, and then to solve the

consequential differential equations that now have a reduction in the number of independent variables. To make all of this work, there are restrictions, however; namely, specific forms for boundary and initial data. This is one of the main reasons for a lack of interest.

In our study, we are considering the above two topics which have such disparate interest. It is our objective to use the evolutionary aspects from group invariance to provide a basis for adaptive motions. Here, we are viewing the invariance properties without regard to the earlier specific boundary and initial conditions, but are primarily concerned with utilizing the variables and the forms which arise solely from the differential equations.

Stefan Feyock

Development of a set of Pascal-based procedures that support both functional programming and Prolog-like deduction has continued. The list manipulation facilities on which these procedures are based can be used to provide a standardized interface among the procedures of the various language implementations. It has become apparent that this integration of language capabilities into a cooperating unit results in a highly synergistic system. LISP-like notation can be used where appropriate, logic programming is available for intelligent database manipulation, and Pascal's control structures can be used to coordinate program flow. Most important, however, is the fact that the Pascal basis on which the system is built allows the higher-level language implementations to interface with any Pascal (-compatible) application, such as simulation programs and database management systems. This allows the addition of deductive capabilities to such programs.

George J. Fix

Work on iterative methods with a special emphasis on spatially varying relaxation parameters is a major thrust. This approach is semi-direct, and the algorithm appears to be well suited to a parallel computing environment.

Collaboration with C. Cox (Clemson University) and the transonic flutter group will continue. The goal here is to study numerical approaches for the full Euler equations. The research will also include the development of appropriately weighted least squares scheme for shocks.

Dennis Gannon, Piyush Mehrotra, and John Van Rosendale

We are presently developing a family of program transformations which will enable compilers to automatically extract parallelism. Our approach is similar to that of David Kuck and colleagues at University of Illinois, and of Fran Allen and others at IBM.

Our work differs from theirs in several ways, including that it is targeted at extracting parallelism from programs written in Blaze, a parallel language developed recently at ICASE. This is considerably easier than finding parallelism in Fortran, since Blaze makes fine grained parallelism explicit and eliminates virtually all of the aliasing problems which hamper attempts to extract parallelism from other high level languages.

The first phase of this project focused on program analysis. In this phase we looked at traditional data flow analysis, classification of data dependencies, and discovery of linear recurrences and sequential loops which could be executed in parallel. This analysis is now largely complete, and we are now looking at issues of parallel run-time environments. Our first target architectures are small shared memory multiprocessors, such as the Flex 32 being acquired at NASA Langley Research Center, and the Alliant computer, which will be the basis of the first prototype of the University of Illinois Cedar computer. Such shared memory multiprocessors are the natural first target for Blaze, though there are many unresolved questions even in this

case. Major research issues include the way in which loops are distributed across processors, the various load balancing questions, and the kind of processor synchronization to use.

James F. Geer

A comparison of pressure coefficients for some two- and three-dimensional slender bodies of simple geometrical shape using standard numerical (panel) methods and uniform asymptotic methods is continuing to try to determine if some of these results can be "pieced together" to describe the forces acting on more complicated geometrical shapes, such as a typical subsonic aircraft. In addition, preliminary work has begun using slender body theory to model a fully three-dimensional wing with a simple planform (e.g., a circle or an ellipse), with special attention being given to the sharp wing tips and the vorticity generated there. The work is being done in collaboration with E. Liu (LaRC) and L. Ting (New York University).

Slender body theory has been used to derive some approximate analytical solutions to the electromagnetic field problem about some simple geometrical shapes. These shapes include a slender body of revolution (to model the fuselage of an aircraft) and a two-dimensional airfoil. The goal of the investigation is to help predict the electromagnetic fields inside an aircraft which is either struck by lightning or experiences a nearby strike. Some of the electromagnetic resonances (eigenvalues) and corresponding mode shapes (eigenfunctions) for perfectly conducting slender bodies of revolution have been determined. Some of these results are now being extended to a dielectric body of revolution. These results will eventually be used to construct the time history (transient) response of a body excited by an impulsive plane wave. This work was motivated by several discussions with F. Pitts (LaRC).

A study of the reduced basis method (a semi-numerical, semi-analytical method which has been used to solve a variety of nonlinear boundary value problems in elasticity) has been started to determine how the method might be applied to some fluid dynamic and scattering problems. Several model problems

are being studied both to understand the method better and to determine its applicability. At present, these model problems include some two-point boundary value problems with boundary layers, some simple exterior scattering problems, and some potential flow problems involving a slender body. The work is being done with C. Anderson (College of William and Mary).

The method of multiple time scales has been implemented using MACSYMA and applied to the problem of determining the transient responses of the van der Pol and Duffing oscillators when the applied force consists of a sum of periodic terms with different frequencies. The conditions under which the system will experience frequency entrainment have been investigated. At present, the results are being extended to more general oscillators; in particular, oscillators for which both the damping and restoring terms are polynomial functions of their arguments.

J. Steven Gibson and I. Gary Rosen

We have been continuing our effort to develop numerical approximation methods for the computation of optimal feedback control gains for infinite dimensional discrete-time linear quadratic regulator problems. Polynomial spline-based schemes for classes of both parabolic systems with boundary control and hereditary systems have been implemented on an IBM PC, tested and observed to perform satisfactorily. The implementation of a scheme using Hermite splines for a problem involving the vibration control of a flexible structure is currently under way.

Chester E. Grosch

A series of calculations (in collaboration with T. Gatski, LaRC) has been initiated whose purpose is to examine the receptivity of the flat plate boundary layer to oscillations in the free stream.

A modification of the two-dimensional Navier-Stokes code of Gatski, Grosch, and Rose is being used to calculate the impulsive start-up of a slender elliptic cylinder. The objective of this work is to study the time evolution of the flow past this slender, blunt-nosed body--particularly the development in time of the separation region at the rear of the body, as a function of slenderness ratio and Reynolds number. The results of the calculation are being compared with the predictions of classical boundary layer theory and with those of triple-deck theory. We also plan to calculate the flow due to the interaction of vortical disturbances in the free stream ahead of the body with the blunt leading edge.

Finally, in collaboration with T. Gatski (LaRC) and M. Rose, a three-dimensional Navier-Stokes code in vorticity and velocity variables using compact schemes is being developed, and will be tested against several analytic solutions.

Max D. Gunzburger and R. A. Nicolaides

Numerical studies of incompressible separated flows are underway using codes implementing finite element methods for the Navier-Stokes equations. For the most part, two types of problems are considered. The first is boundary layer flows over irregular obstacles such as ramps, curved ramps, steps, cavities, and combinations of these. Here a careful study of the effects of outflow boundary conditions has been carried out. The purpose of these calculations is to study the effects of the various obstacles on separation and, hopefully, to predict the appearance of transition regions. Calculations have been performed for a variety of cases, and one may conclude that the numerical simulation can indeed be used for the intended purpose. The second project is the calculation of flows around airfoils at high angles of attack. A study of turbulence models which may be incorporated into the finite element codes in an efficient manner has been carried out. A finite element method which incorporates an algebraic turbulence model has been rigorously analyzed and shown to converge. In addition to the above personnel, the project has involved students at Carnegie-Mellon University.

Subramaniya I. Hariharan

Nonlinear acoustic wave propagation in atmosphere is being studied. Both theoretical and numerical studies are being made. Currently study of accurate absorbing boundary conditions is underway. Stability of these conditions is also being studied together with computational verifications. Verifications are done using a linear analytic model.

Computational methods for inverse problems, particularly in shape detection, are being developed. These methods incorporate singular integral equation methods with regularization techniques. Possibilities of extending this method with varying index of refractions (inhomogeneous) bodies are also explored.

Efficient computational techniques for wave propagation in wave guides and ducts are being developed. This work is a continuation of the work done with H. Lester (LaRC).

Murshed Hossain

High Reynolds number turbulent shear flows have a great range of temporal and spatial scales. It is almost impossible to simulate them on presently available or projected future computers. Large eddy simulation (LES) provides a viable alternative. This is based on the assumption that the velocity field can be divided into large and small eddies and the motions of the large eddies are not sensitive to the details of the small eddies (smaller than the grid size of a sufficiently fine mesh). The small eddies are assumed to have a universal character (there is evidence to this effect) and hence are amenable to modelling. This is called the subgrid scale modelling (SGS). The purpose of the present study is to estimate the eddy-viscosity by systematic removal of small scales from the dynamics using a renormalization technique. This work is in progress in collaboration with George Vahala and Ye Zhou (William and Mary). Preliminary results will be presented at the 1985 Sherwood Theory Conference to be held on April 15-17, 1985, in Madison, Wisconsin.

It is well known that free stream turbulence, entropy disturbance in tunnel acoustic field, triggers unstable waves in a boundary layer. But the mechanism by which an external disturbance environment enters the boundary layer (and the nature of its signature in the perturbed flow) are not well understood. The object of the present research effort is to perform controlled numerical experiments to get some insight into these mechanisms. With this purpose in view, we are constructing an algorithm for VPS-32 for solving three dimensional Navier-Stokes equations. Among the physical problems we intend to study are: response of a boundary layer to a stationary or moving acoustic wave and convected array of counter rotating vortices. So far we have an explicit code validated against the linear theory. An internal report is in preparation with a purpose that other individuals will be able to use this code if they wish.

M. Yousuff Hussaini

The program of research in hydrodynamic stability and transition to turbulence is continuing. A new spectral algorithm was implemented to solve three-dimensional Navier-Stokes equations with periodicity assumptions in the horizontal direction (ICASE Report No. 85-19, NASA CR 172561), and numerical experiments were carried out to verify the perturbation theories related to subcritical transition to turbulence in plane Poiseuille flow and Blasius boundary layer flow (AIAA-85-0296). Relative advantages of LFC techniques such as heating, suction, and pressure gradient are being investigated. Also, new algorithms have been developed to treat the problems of Rayleigh-Benard convection and Taylor-Couette flow in finite cylinders.

Numerical simulations of two-dimensional viscous compressible flows have been performed to verify the effectiveness of a control surface in the outer part of the boundary layer to bounce off the shock, thus preventing shock-induced separation of flow (AIAA Paper No. 85-0523).

In another study, the eddy shocklets observed in high speed free shear layers are modelled. A subsonically convecting eddy is injected into a

supersonic stream. The subsequent shocklet formation and eddy deformation is simulated with a view to verify if the shocklet-induced eddy deformation provides the explanation for decrease in entrainment rate at high Mach numbers.

The feasibility of spectral methods to handle chemically reacting supersonic flows was tried out in the case of a quasi one-dimensional problem. Further study is planned of laminar flame propagation problems including flame front interaction with shock waves and turbulence.

These studies are carried out in collaboration with D. Bushnell (LaRC), J. P. Drummond (LaRC), C. Streett (LaRC), and T. Zang (LaRC).

Kazufumi Ito and Robert K. Powers

The solution of infinite dimensional linear-quadratic regulator problems is often sought in feedback form. The feedback gain is usually calculated via an operator Riccati equation. For systems with bounded input and output it has been shown that an alternative set of equations, known as the Chandrasekhar equations, may be solved to obtain the gain. Furthermore, for certain classes of problems the numerical solution of the Chandrasekhar equations is computationally more efficient than approximation of the Riccati operator. Investigations into the unbounded input/output case are being made since many realistic physical control problems (i.e., boundary control and observation) fall in this category. In addition, the features of the Chandrasekhar equations which make them computationally attractive are present in boundary control and observation of distributed parameter systems.

David A. Kopriva

Research continues on the use of spectral multidomain methods for inviscid gas-dynamics problems. Linear scalar and system tests show that stability and spectral accuracy can be retained with a very simple procedure. The method

has also been applied to a nonlinear quasi-one-dimensional nozzle flow, and results show that the error is spectral. The main advantage to the multi-domain solution of this type of problem is that larger time steps can be used for a given number of grid points. A code to test the method on the two-dimensional Ringleb flow is now being developed.

Research on shock fitting methods is also continuing. The problem of shock detection has usually required a user to specify an arbitrary parameter. In joint work with S. Davis ideas from the theory of total variation diminishing (TVD) schemes for hyperbolic systems are being applied to the problem of how to detect a shock without requiring problem dependent parameters.

Gunilla Kreiss

A time-dependent, one-dimensional model equation of gas dynamics containing a dissipative term is being considered. This problem has a unique steady solution. In the case of a small dissipative constant, it is difficult to compute this steady solution. To understand why this is so, the corresponding eigenvalue problem has been explored. The result of this analysis shows that there is only one very small eigenvalue which causes the difficulties. Since it is a single eigenvalue, the convergence can be speeded by extrapolation techniques. Numerical experiments are being done.

William D. Lakin

Integrating matrices based on sliding subgrids provide the basis for a fast and efficient numerical procedure for solving the eigenvalue problems associated with the vibrations and buckling of rotating flexible beams with cantilevered boundary conditions. Such beams provide a model for helicopter rotor blades. However, for beams with non-cantilevered boundary conditions, integrating matrices alone are not sufficient to formulate the required matrix

eigenvalue problem, and, in general, both differentiating and boundary matrices must also be utilized. Previous versions of this type of differentiating matrix have been restricted to uniform grids and have had large approximation errors at endpoints which make them unsuitable for computation. A generalized differentiating matrix was developed which can approximate differential operators on arbitrary grids. Inclusion of near boundary points in a grid was shown to dramatically reduce approximation error at endpoints.

The integrating and generalized differentiating matrices are now being used to obtain the numerical solutions at boundary value problems for rods with non-cantilevered boundary conditions. The method is also being generalized to two dimensions to deal with the vibrations of helicopter rotors modeled as thin elastic shells.

Liviu Lustman

Work is continuing on compact schemes applied to elasticity problems. A vector processor code is being developed, which is designed to solve the full tri-dimensional static elasticity equations for composite materials, for simple geometrical configurations. Because of inherent properties of the compact scheme, the relaxation procedure acts separately on three sets of mesh points, which introduces interesting parallel computation possibilities. The code aims at modelling experiments such as failure tests for composite materials. This work has been performed in collaboration with M. E. Rose and in coordination with J. Stroud (LaRC).

A tutorial paper, "A Review of Spectral Methods," has been prepared and presented at the "Short Course on Numerical Methods for Partial Differential Equations," University of Tennessee Space Institute, Tullahoma, TN, March 1985.

Joint research with D. Ebin (SUNY at Stony Brook) is continuing on incompressible inviscid flow modelling in two- and three-dimensions.

Mala Mehrotra and John Van Rosendale

In recent months we have completed a simulation study of the mapping of tree search algorithms to loosely coupled architectures. This study concentrated on the effects of various heuristic load balancing strategies which can achieve high utilization without incurring excessive communications costs. A natural extension of this research would be to study the problem of mapping functional programming languages onto non-shared memory architectures. During the summer we plan to study this problem by writing a Lisp based interpreter for a subset of the Blaze language. A major issue here is the distribution of large data structures, such as arrays, across the local memories of the processors in the architecture. No adequate approach to this problem has yet been discovered, but a number of promising approaches are being explored.

Piyush Mehrotra and John Van Rosendale

We have recently designed a parallel programming language, Blaze, intended for scientific programming. Our language resembles conventional programming languages but uses applicative procedure calls, which allow compilers to automatically extract coarse-grained parallelism. The first version of Blaze has now been frozen and is being implemented. We are also formulating a denotational semantics description of the language, which is clearly necessary, since the semantics of the "forall" loops here is quite subtle and requires careful specification.

During the process of formulating a denotational description of Blaze, we are also looking at a number of possible extensions to the language. One of these is an interface to Fortran programs and subroutine libraries. The development of such an interface is obviously important, because of the large amount of existing scientific programs in Fortran. However, it is also quite difficult, since many features of Fortran, such as equivalence statements and common blocks, introduce severe aliasing.

Another area in which we hope to extend Blaze is in the computational model embedded in Blaze. The current version of Blaze is entirely determinate. In most cases determinate execution is highly desirable, but there are circumstances where asynchronous or indeterminate execution could yield higher utilization and improved performance. We would like to introduce some form of controlled asynchrony in Blaze, allowing the run time environment to select the execution order, while retaining determinate execution. The precise details of this are still being formulated.

Vijay K. Naik and Joel H. Saltz

There are numerous problems involving time dependent partial differential equations for which obtaining a relatively accurate solution can be an expensive, time consuming process. In many algorithms for the solution of such time dependent problems it is necessary to solve a sequence of linear equations involving the same coefficient matrix but different "right-hand side." The "right-hand sides" of equations corresponding to the consecutive steps are dependent on the solutions of the equations corresponding to the earlier time steps in the sequence.

Our research work is aimed at discovering how to solve these problems efficiently on multiprocessors. One of the factors that reduces the efficiency of multi-processor algorithms and limits the number of processors that may be usefully employed is the amount and the timing of communication that must take place between problem partitions that run on different processors. Iterative algorithms that involve partitioning the domain of the partial differential equation and with each partition sweeping over several time steps reduce synchronization requirements and allow overlap of computation and communication. The performance implications of this communication and computation overlap varies with the architecture of the multi-processor system. Similarly the hardware requirements vary for various communication and computation overlap strategies. These issues are currently being analyzed. Performance models are being developed for some existing MIMD

architectures as well as for some hypothetical systems. The scheduling of various processes and the dynamic load balancing of these processes on the available processors are the other issues that are under investigation.

Vijay K. Naik and Shlomo Ta'asan

Algorithms based on multigrid techniques are among the most efficient methods for solving partial differential equations. On a sequential machine, a wide class of problems discretized on a grid with n points requires only $O(n)$ arithmetic operations to obtain a solution to within the truncation error of the discretization. This makes the multigrid methods optimal on the sequential machines. This optimal property, together with the fact that many aspects of the multigrid algorithms are highly parallelizable, make these methods attractive for implementation on multi-processor systems. Several researchers have studied the effects of parallelizing the intra-grid and inter-grid operations. But it is not very clear if the optimality observed on sequential machines is conserved in space and in the number of processors when these methods are implemented on multi-processors. The work undertaken here is to explore this question further for shared and non-shared memory architectures. The effort is aimed at studying the effects of various communication strategies and also at understanding the effects of various implementations on the convergence rates. We are also studying the advantages and disadvantages of using a large number of simple processors and those of using a small number of powerful processors. The immediate objective is to develop accurate performance models of various parallel algorithms for the currently available MIMD multi-processor systems such as the FLEX/32.

Vijay K. Naik and John Van Rosendale

An examination of numerical programs indicates that most of the available parallelism is concentrated at the loop level, rather than at the procedure

level. One of the recent innovations in vector computers is "scatter-gather" hardware, which allows general permutations of data, thereby broadening the class of loops which can be performed efficiently. But for many types of loops the ability to permute data is not sufficient. For example, the computation of the product of a sparse matrix and a vector cannot be done easily on a vector computer, even if scatter-gather hardware is available.

A natural generalization of permutation is the "replace-add" or "fetch-add" operation of the NYU Ultracomputer. This operation allows many processors in a multiprocessor system to access and update semaphores in parallel. Many numerical problems, including sparse matrix problems and particle-in-cell plasma simulations, require exactly this type of operation. But "replace-add" hardware is probably not the complete answer since, for one thing, the size of problem which can be solved is limited by the size of the "replace-add" network available. As an alternative, we are studying the use of single-stage multi-microprocessor networks which can be used to emulate a "replace-add" network of arbitrary size. Simulation results obtained indicate that this approach reduces or eliminates load balancing problems and that the use of a single-stage network used in this way may be more attractive than the use of Log-stage networks, such as the Omega network. Modelling and performance analysis of such systems is currently under way.

Robert E. Noonan

Work in porting the Mystro system to the VAX was completed. After some experimentation with syntactic error recovery, it was decided to use a Mystro parser in the implementation of BLAZE. In order to simplify conversion of the existing YACC grammar for BLAZE, several enhancements were added to Mystro, including the use of precedence and associativity to simplify the subgrammar for arithmetic expressions.

Work was undertaken to use a grammar as a technique for specifying menus and their associated actions. The application investigated was the user

interface for a software code management system (SCMS). At this time, a number of activities related to Space Station can apply this technology.

Research continues on applying table-driven code generation techniques to flexible architecture machines involving many processors. The problems posed thus far seem to be solvable by a three-step process, involving a machine-dependent code improver, a code generator, and a peephole optimizer. All three processes would be table-driven and all three could be derived from a single machine description.

Robert E. Noonan and Nancy E. Shoemaker

Scientists at ICASE often do much of their computer work on the VAX. However, many mathematical programs are best run on the central computing complex, either on the Cybers or on the VPS (nee Cyber 203). This has meant that ICASE scientists have had to learn at least two distinct computer command languages and conventions. Using the VPS is particularly complicated because a Cyber job must be used to generate the VPS job, which in turn must generate a Cyber job to distribute the output back to the VAX; in addition, the command language for the VPS is distinct from that of the Cybers.

Until recently, the solution to this problem has been to develop Unix scripts specifically tailored to the needs of each individual scientist. Over the last two months work has been progressing on the development of menu-driven programs to generate batch jobs, one for the Cybers and one for the VPS, to help minimize this complexity.

The programs are unusual in that they are merely LR(1) parsers for the grammar describing the needed menus and associated actions. Most of the difficulty in developing these programs came from trying to understand the command languages of the target machines. The programs themselves are an interesting application of LR parsing technology.

Merrell L. Patrick

Computing systems of the future for large scale scientific and engineering computations will consist of many processors and memories working in parallel to solve a single problem. Efficient use and ease of use of these future systems are two basic problems facing potential users. The development of new parallel algorithms, parallel execution time models which predict the performance of the algorithms on different parallel architectures, and parallel programming environments for expressing the algorithms are essential for progress toward the solution of these problems.

In collaboration with Daniel Reed (University of Illinois) the applicability of static data flow architectures to the iterative solution of sparse linear systems of equations is under investigation. An analytic performance model of a static data flow computation has been developed. This model includes both spatial parallelism, concurrent execution in multiple PEs, and pipelining, the streaming of data from array memories through the PEs. The performance model is being used to analyze the performance of a row partitioned, iterative algorithm for solving sparse linear systems of algebraic equations. Based on the results of this analysis, design parameters for the static data flow architecture as a function of matrix sparsity and dimension are proposed.

In collaboration with J. Cuny (University of Massachusetts), D. Gannon (Purdue), M. Gokhale (University of Delaware), P. Mehrotra (Purdue), T. Pratt (University of Virginia), J. Van Rosendale, and R. Voigt, work is in progress on trying to define the essential ingredients of parallel programming languages for scientific computations. The suitability of different programming paradigms, e.g., communicating sequential processes, functional programming, are being studied. Dimensions of programming languages for expressing parallelism in scientific computations are being defined. These include appropriate data objects, operations, program control structures, and data control mechanisms.

Finally a new study has begun with L. Adams (UCLA) to determine effects that different forms of iteration matrices have on communication requirements of parallel algorithms for solving sparse linear systems.

Merrell L. Patrick and Terrence W. Pratt

Several programs for the iterative solution of random, sparse linear systems have been developed, using Pisces Fortran and the PISCES parallel programming environment. The system is solved by use of several cooperating parallel tasks that each compute a portion of the solution vector. The various programs differ primarily in the manner in which communication among the parallel tasks is organized: broadcast, pairwise among all pairs, pairwise among the minimal number of pairs, or pipelined data flow. Asynchronous as well as synchronous versions (synchronization at the end of each iteration) have been programmed. Studies are continuing of the amount of communication (number and size of messages) in the various versions and the effect on convergence of asynchronous operation.

Robert K. Powers

Research is continuing on the approximation of feedback gains for linear hereditary control systems. Numerical studies using an averaging approximation scheme have demonstrated that the Chandrasekhar equations results in a significant reduction of computer time over solution of the gain via Riccati equations. Application of the equations to higher order approximation schemes is underway. Also, possible application to distributed parameter systems will be investigated.

In joint work with K. Ito (Brown University), infinite dimensional versions of the Chandrasekhar equations are being developed for systems with unbounded input/output. In particular, applications to boundary control and observation are sought.

Research is also continuing in collaboration with J. Burns (VPI & SU) on hereditary models for active flutter control of a thin airfoil and on control of hybrid distributed parameter systems.

Terrence W. Pratt

The PISCES parallel programming environment allows the scientific programmer to write parallel programs that are intended to run on various parallel architectures. Programming is in PISCES Fortran (an extension of Fortran 77) under the Unix operating system. Several "granularities" of parallel operations are provided.

The PISCES environment has been implemented on the ICASE VAX 750 and on a network of Apollo Domain workstations at the University of Virginia. An implementation for the Flexible Corp. FLEX/32 at NASA Langley is being designed, with implementation planned for summer 1985.

Milton E. Rose

In joint work with T. Gatski (LaRC) and C. Grosch (ODU) a finite difference method to solve the time dependent incompressible three-dimensional Navier-Stokes equations is being studied. The underlying construction employs separate local solution bases for the velocity and vorticity fields. A novel locally one-dimensional splitting method is employed to treat the vorticity transport-diffusion equations.

With L. Lustman and S. Ta'asan compact finite difference equations are being studied to treat the equilibrium of an n-ply rectangular plate. Simple SOR techniques are being examined with the purpose of laying the groundwork for developing multigrid methods.

Shlomo Ta'asan

The development of fast solvers for nonlinear equation near bifurcation or limit points is being studied. Usual multigrid methods which do not include a continuation process will fail to work when applied to such problems. The reason for this is that the linearized equations are close to singularity and

coarse grids do not approximate well fine grids for some smooth functions. Essentially the same difficulty exists for (linear) slightly indefinite problems. An efficient multigrid algorithm was developed for the latter (A. Brandt and S. Ta'asan) and is now being extended to nonlinear problems including solution near singular points. Numerical experiments are being done with a vortex breakdown problem with A. Brandt (Weizmann Institute).

A multigrid treatment of compact finite element schemes is the subject of another study. Numerical experiments with the Poisson equation and the elasticity equations have been done, both with Dirichlet type boundary conditions. A solution accurate to the level of truncation errors was obtained by, at most, two multigrid cycles. The next step in the development will be to get the same efficiency with non-Dirichlet boundary conditions.

Application of a previously developed idea for quasi-elliptic schemes (A. Brandt and S. Ta'asan) to incompressible Navier-Stokes equations with velocity-vorticity variables in two-dimensions is being done. Preliminary experiments with periodic boundary conditions show the usual multigrid behavior, i.e., solution accurate to the level of truncation errors is obtained in just two multigrid cycles. Work is being done to obtain this efficiency for other types of boundary conditions including problems which model flow with separation. This work was motivated by discussions with M. Rose, C. Grosch (ODU), M. Salas (LaRC), and M. Hafez (Computer Dynamics, Inc.).

Eli Turkel

Work continues on numerical solutions to the Helmholtz equation. An ICASE report was issued together with J. Gozani (Tel-Aviv University) and A. Nachshon (Tel-Aviv University) "On a combined conjugate gradient - multigrid iterative method." The Helmholtz equation is solved in the least square sense by the conjugate gradient method. The preconditioning is based on a partial inverse of the Laplacian based on a subset of multigrid. Other

work was done with A. Bayliss (Exxon Corporate Research) and C.I. Goldstein (Brookhaven National Laboratory) in an ICASE report analyzing the accuracy of discretizations for wave-like equations. It was found that the number of points per wavelength is not a sufficient measure to describe the accuracy of a scheme. Finally in a third ICASE report we further analyze preconditionings for the Helmholtz equation, especially the number of levels of multigrid that leads to the best results. This report also contains applications to underwater acoustics. A talk describing these results was given by C. I. Goldstein at a conference on underwater acoustics.

A second ongoing project is joint work with A. Bayliss, L. Maestrello (LaRC), and P. Parikh (Vigyan Research Associates, Inc.). We are analyzing the time-dependent behavior of a boundary layer over a flat plate when excited by a time harmonic inflow boundary condition. The profile of the inflow perturbation is found by calculating an unstable mode for the Orr-Sommerfeld equation. The nonlinear growth of the boundary layer is then calculated by numerically solving the full compressible laminar Navier-Stokes equations. A fourth-order scheme in space is used to correctly calculate the growth rates. As a related project we also consider the control of the growing mode by heating elements on the flat plate. Using a fluctuating heat and/or cooling source a control can be found. Extensions to three dimensions is presently under way. An ICASE report has been issued and another is being written.

The third project is the numerical solution of the steady state compressible Euler and Navier-Stokes equations about aerodynamic bodies. The existing Runge-Kutta code has been extended to include the thin layer Navier-Stokes equation using an eddy viscosity turbulence model. An ICASE report has been written together with C. Swanson (LaRC). Extensions to three dimensions are being carried out by V. Vatson (LaRC). Work was also done on improving the time step for viscous calculations using a Crocco type scheme. Work is beginning on the analysis of schemes when nonuniform grids are used and an ICASE report is in preparation. Finally work is continuing on the use of these codes for slow flow without losing the fast convergence of the schemes to the steady-state. Both analysis and computations are being pursued. One ICASE report has already appeared on this subject.

Robert G. Voigt

Preparation of an extensive review of the state of parallel numerical algorithms for partial differential equations has been completed in collaboration with J. Ortega (University of Virginia). The work includes an overview of the architectural issues of parallel and vector computers that influence algorithm performance. Both direct and iterative techniques are considered along with an indication of the kinds of applications that have been addressed. An extensive bibliography is also included.

Another effort with J. Olinger (Stanford) involves studying the nature of high performance scientific computing. This involves many stages and disciplines: problem definition--engineering and the sciences; mathematical formulation--engineering, the sciences, and applied mathematics; discretization and algorithm formulation--numerical and algorithmic analysis; algorithm description and implementation--computer languages and systems; execution of the calculation--computer hardware; and interpretation of the results--data base management, graphics, etc. A central theme is that synergism between these phases and disciplines is necessary to produce a modern computational environment; that is, one which can be easily used, employs modern technology, exploits parallelism to a high degree, and utilizes sophisticated, efficient algorithms. Several other researchers have been asked to write on various aspects of the synergistic process, and the result is intended as a volume in the SIAM Frontiers of Applied Mathematics series.

REPORTS AND ABSTRACTS

October 1, 1984 through March 31, 1985

Canuto, C.: *Boundary Conditions in Chebyshev and Legendre Methods.* ICASE Report No. 84-52, October 1, 1984, 38 pages. Submitted to SIAM J. Numer. Anal.

We discuss two different ways of treating non-Dirichlet boundary conditions in Chebyshev and Legendre collocation methods for second order differential problems.

An error analysis is provided. The effect of preconditioning the corresponding spectral operators by finite difference matrices is also investigated.

Roe, P. L.: *Generalized formulation of TVD Lax-Wendroff schemes.* ICASE Report No. 84-53, October 23, 1984, 14 pages.

The work of Davis [1] which imports the concept of total-variation-diminution (TVD) into non-upwinded, Lax-Wendroff type schemes is reformulated in a way which is easier to analyze. The analysis reveals a class of TVD schemes not observed by Davis.

Bokhari, S. H.: *Shuffle-exchanges on augmented meshes.* ICASE Report No. 84-54, October 24, 1984, 12 pages.

Prior research has shown how a mesh connected array of size $N = 2^K$, K an integer, can be augmented by adding at most one edge per node such that it can perform a shuffle-exchange of size $N/2$ in constant time.

We now show how to perform a shuffle-exchange of size N on this augmented array in constant time. This is done by combining the available perfect shuffle of size $N/2$ with the existing nearest neighbor connections of the mesh. By carefully scheduling the different permutations that are composed in order to achieve the shuffle, the time required is reduced to 5 steps, which is shown to be optimal for this network.

Goodman, J. B. and R. J. LeVeque: *A geometric approach to high resolution TVD schemes*. ICASE Report No. 84-55, October 29, 1984, 35 pages. Submitted to SIAM J. Numer. Anal.

We use a geometric approach, similar to Van Leer's MUSCL schemes, to construct a second-order accurate generalization of Godunov's method for solving scalar conservation laws. By making suitable approximations we obtain a scheme which is easy to implement and total variation diminishing. We also investigate the entropy condition from the standpoint of the spreading of rarefaction waves. For Godunov's method we obtain quantitative information on the rate of spreading which explains the kinks in rarefaction waves often observed at the sonic point.

Tin-Chee Wong, C. H. Liu, and J. Geer: *Comparison of uniform perturbation solutions and numerical solutions for some potential flows past slender bodies*. ICASE Report No. 84-56, October 29, 1984, 32 pages. To appear in Computers & Fluids.

Approximate solutions for potential flow past an axisymmetric slender body and past a thin airfoil are calculated using a uniform perturbation method and then compared with either the exact analytical solution or the solution obtained using a purely numerical method. The perturbation method is based upon a representation of the disturbance flow as the superposition of singularities distributed entirely within the body, while the numerical (panel) method is based upon a distribution of singularities on the surface of the body. It is found that the perturbation method provides very good results for small values of the slenderness ratio and for small angles of attack. Moreover, for comparable accuracy, the perturbation method is simpler to implement, requires less computer memory, and generally uses less computation time than the panel method. In particular, the uniform perturbation method yields good resolution near the regions of the leading and trailing edges where other methods fail or require special attention.

Salas, M. D., S. Abarbanel and D. Gottlieb: *Multiple steady states for characteristic initial value problems*. ICASE Report No. 84-57, November 1, 1984, 43 pages. Submitted to J. Comput. Phys.

The time dependent, isentropic, quasi-one-dimensional equations of gas dynamics and other model equations are considered under the constraint of characteristic boundary conditions. Analysis of the time evolution shows how different initial data may lead to different steady states and how seemingly anomalous behavior of the solution may be resolved. Numerical experimentation using time consistent explicit algorithms verifies the conclusions of the analysis. The use of implicit schemes with very large time steps leads to erroneous results.

Rose, Milton E.: *A compact finite element method for elastic bodies.* ICASE Report No. 84-58, November 7, 1984, 38 pages. To appear in *J. Numer. Meth. for PDEs*.

A nonconforming finite element method is described for treating linear equilibrium problems, and a convergence proof showing second order accuracy is given. The close relationship to a related compact finite difference scheme due to Phillips and Rose [2] is examined. A condensation technique is shown to preserve the compactness property and suggests an approach to a certain type of homogenization.

Lustman, L.: *A review of spectral methods.* ICASE Report No. 84-59, November 19, 1984, 25 pages. *Numerical Methods for Partial Differential Equations*, S. I. Hariharan and T. H. Moulden (eds.), January 1985.

This paper presents a brief outline of spectral methods for partial differential equations. The basic ideas, together with simple proofs are discussed. An application to potential transonic flow is also reviewed.

Hussaini, M. Y. and W. D. Lakin: *Existence and non-uniqueness of similarity solutions of a boundary layer problem.* ICASE Report No. 84-60, November 21, 1984, 17 pages. Submitted to *Quart. J. Mech. Appl. Math.*

This work considers a Blasius boundary value problem with inhomogeneous lower boundary conditions $f(0) = 0$ and $f'(0) = -\lambda$ with λ strictly positive. The Crocco variable formulation of this problem has a key term which changes sign in the interval of interest. It is shown that solutions of the boundary value problem do not exist for values of λ larger than a positive critical value λ^* . The existence of solutions is proved for $0 < \lambda < \lambda^*$ by considering an equivalent initial value problem. However, for $0 < \lambda < \lambda^*$, solutions of the boundary value problem are found to be nonunique. Physically, this non-uniqueness is related to multiple values of the skin friction.

Bayliss, A., Maestrello, L. and Turkel, E.: *On the interaction of a sound pulse with the shear layer of an axisymmetric jet, III. Nonlinear effects.* ICASE Report No. 84-61 November 23, 1984, 22 pages. Submitted to *J. Sound Vib.*

The fluctuating field of a jet excited by transient mass injection is simulated numerically. The model is developed by expanding the state vector as a mean state plus a fluctuating state. Nonlinear terms are not neglected, and the effect of nonlinearity is studied. A high order numerical method is used to compute the solution. The results show a

significant spectral broadening in the flow field due to the nonlinearity. In addition, large scale structures are broken down into smaller scales.

Swanson, R. C. and E. Turkel: *A multistage time-stepping scheme for the Navier-Stokes equations*. ICASE Report No. 84-62, November 23, 1984, 28 pages. AIAA Paper No. 85-0035 presented at the AIAA Aerospace Science Meeting, January 14-17, 1985, Reno, NV.

A class of explicit multistage time-stepping schemes is used to construct an algorithm for solving the compressible Navier-Stokes equations. Flexibility in treating arbitrary geometries is obtained with a finite-volume formulation. Numerical efficiency is achieved by employing techniques for accelerating convergence to steady state. Computer processing is enhanced through vectorization of the algorithm. The scheme is evaluated by solving laminar and turbulent flows over a flat plate and an NACA 0012 airfoil. Numerical results are compared with theoretical solutions or other numerical solutions and/or experimental data.

Brenier, Y. and S. Osher: *Approximate Riemann solvers and numerical flux functions*. ICASE Report No. 84-63, December 5, 1984, 33 pages. Submitted to SIAM J. Numer. Anal.

Given a monotone function $z(x)$ which connects two constant states, $u_L < u_R$, ($u_L > u_R$), we find the unique (up to a constant) convex (concave) flux function, $\hat{f}(u)$, such that $z(x/t)$ is the physically correct solution to the associated Riemann problem. For $z(x/t)$, an approximate Riemann solver to a given conservation law, we derive simple necessary and sufficient conditions for it to be consistent with any entropy inequality. Associated with any member of a general class of consistent numerical fluxes, $h_f(u_R, u_L)$, we have an approximate Riemann solver defined through $z(\zeta) = (-d/d\zeta) h_{f_\zeta}(u_R, u_L)$ where $f_\zeta(u) = f(u) - \zeta u$. We obtain the corresponding $\hat{f}(u)$ via a Legendre transform and show that it is consistent with all entropy inequalities iff $h_{f_\zeta}(u_R, u_L)$ is an E flux for each relevant ζ . Examples involving commonly used two point numerical fluxes are given, as are comparisons with related work.

Hall, P. and M. R. Malik: *On the instability of a three-dimensional attachment line boundary layer: Weakly nonlinear theory and a numerical approach*. ICASE Report No. 84-64, December 6, 1984, 65 pages. Submitted to J. Fluid Mech.

The instability of a three-dimensional attachment line boundary layer is considered in the nonlinear regime. Using weakly nonlinear theory, it is found that, apart from a small interval near the (linear) critical Reynolds number, finite amplitude solutions bifurcate subcritically from the upper branch of the neutral curve. The time-dependent Navier-Stokes equations for the attachment line flow have been solved using a Fourier-Chebyshev spectral method, and the subcritical instability is found at wavenumbers that correspond to the upper branch. Both the theory and the numerical calculations show the existence of supercritical finite amplitude (equilibrium) states near the lower branch which explains why the observed flow exhibits a preference for the lower branch modes. The effect of blowing and suction on nonlinear stability of the attachment line boundary layer is also investigated.

Fix, G. J. and M. Suri: *Three-dimensional mass conserving elements for compressible flows*. ICASE Report No. 84-65, December 13, 1984, 27 pages. To appear in Comput. Math. Appl.

A variety of finite element schemes has been used in the numerical approximation of compressible flows particularly in underwater acoustics. In many instances instabilities have been generated due to the lack of mass conservation. In this paper we develop new two- and three-dimensional elements which avoid these problems.

Banks, H. T. and J. M. Crowley: *Estimation of material parameters in elastic systems*. ICASE Report No. 84-66, December 28, 1984, 45 pages. Submitted to Matematica Aplicada e Computacional.

In this paper we present theoretical and numerical results for inverse problems involving estimation of spatially varying parameters such as stiffness and damping in distributed models for elastic structures such as Euler-Bernoulli beams. An outline of algorithms we have used and a summary of some of our computational experiences are presented.

Ito, K. and R. K. Powers: *Chandrasekhar equations for infinite dimensional systems*. ICASE Report No. 84-67, December 31, 1984, 36 pages. Submitted to SIAM J. Control Optim.

In this paper we derive the Chandrasekhar equations for linear time invariant systems defined on Hilbert spaces using a functional analytic technique. An important consequence of this is that the solution to the evolutionary Riccati equation is strongly differentiable in time, and one

can define a 'strong' solution of the Riccati differential equation. A detailed discussion on the linear quadratic optimal control problem for hereditary differential systems is also included.

Ortega, J. M. and R. G. Voigt: *Solution of partial differential equations on vector and parallel computers.* ICASE Report No. 85-1, January 2, 1985, 173 pages. To appear in SIAM Review.

In this paper we review the present status of numerical methods for partial differential equations on vector and parallel computers. A discussion of the relevant aspects of these computers and a brief review of their development is included, with particular attention paid to those characteristics that influence algorithm selection. Both direct and iterative methods are given for elliptic equations as well as explicit and implicit methods for initial-boundary value problems. The intent is to point out attractive methods as well as areas where this class of computer architecture cannot be fully utilized because of either hardware restrictions or the lack of adequate algorithms. A brief discussion of application areas utilizing these computers is included.

Voigt, R. G.: *Where are the parallel algorithms?* ICASE Report No. 85-2, January 16, 1985, 14 pages. Submitted to the 1985 National Computer Conference, AFIPS NCC Proceedings.

Four paradigms that can be useful in developing parallel algorithms are discussed. These include computational complexity analysis, changing the order of computation, asynchronous computation, and divide and conquer. Each is illustrated with an example from scientific computation, and it is shown that computational complexity must be used with great care or an inefficient algorithm may be selected.

Gottlieb, D. and E. Tadmor: *Recovering pointwise values of discontinuous data within spectral accuracy.* ICASE Report No. 85-3, January 31, 1985, 20 pages. Proc. of "The Impact of Supercomputers in the Next Decade of CFD," Jerusalem, December 1984.

We show how pointwise values of a function, $f(x)$, can be accurately recovered either from its spectral or pseudospectral approximations, so that the accuracy solely depends on the local smoothness of f in the neighborhood of the point x . Most notably, given the equidistant function grid values, its intermediate point values are recovered within spectral accuracy, despite the possible presence of discontinuities scattered in the domain. (Recall that the usual spectral convergence rate decelerates otherwise to first order, throughout.)

To this end we employ a highly oscillatory smoothing kernel, in contrast to the more standard positive unit-mass mollifiers.

In particular, post-processing of a stable Fourier method applied to hyperbolic equations with discontinuous data, recovers the exact solution modulo a spectrally small error. Numerical examples are presented.

Noonan, R. E.: *An algorithm for generating abstract syntax trees.* ICASE Report No. 85-4, January 31, 1985, 18 pages. Submitted to Computer Languages.

In this paper, we discuss the notion of an abstract syntax. An algorithm is presented for automatically deriving an abstract syntax directly from a BNF grammar. The implementation of this algorithm and its application to the grammar for Modula are discussed.

Lakin, W. D.: *Differentiating matrices for arbitrarily spaced grid points.* ICASE Report No. 85-5, January 31, 1985, 23 pages. Submitted to Internat. J. Numer. Methods Engrg.

Differentiating matrices allow the numerical differentiation of functions defined at points of a discrete grid. The present work considers a type of differentiating matrix based on local approximation on a sequence of sliding subgrids. Previous derivations of this type of matrix have been restricted to grids with uniformly spaced points, and the resulting derivative approximations have lacked precision, especially at endpoints. The new formulation allows grids which have arbitrarily spaced points. It is shown that high accuracy can be achieved through use of differentiating matrices on non-uniform grids which include "near-boundary" points. Use of the differentiating matrix as an operator to solve eigenvalue problems involving ordinary differential equations is also considered.

Fleming, P. J.: *SUBOPT - A CAD program for suboptimal linear regulators.* ICASE Report No. 85-6, February 4, 1985, 16 pages. Proc. Institute of Measurement and Control Workshop on Computer-Aided Control System Design, Brighton, England, September 1984, pp. 13-20.

This interactive software package provides design solutions for both standard linear quadratic regulator (LQR) and suboptimal linear regulator problems. Intended for time-invariant continuous systems, the package is easily modified to include sampled-data systems. LQR designs are obtained by established techniques while the large class of suboptimal problems containing controller and/or performance index options is solved using a

robust gradient minimization technique. Numerical examples demonstrate features of the package and recent developments are described.

Banks, H. T. and I. G. Rosen: *A Galerkin method for the estimation of parameters in hybrid systems governing the vibration of flexible beams with tip bodies.* ICASE Report No. 85-7, February 5, 1985, 44 pages. Submitted to J. Math. Anal. Appl.

In this report we develop an approximation scheme for the identification of hybrid systems describing the transverse vibrations of flexible beams with attached tip bodies. In particular, problems involving the estimation of functional parameters (spatially varying stiffness and/or linear mass density, temporally and/or spatially varying loads, etc.) are considered. The identification problem is formulated as a least squares fit to data subject to the coupled system of partial and ordinary differential equations describing the transverse displacement of the beam and the motion of the tip bodies respectively. A cubic spline-based Galerkin method applied to the state equations in weak form and the discretization of the admissible parameter space yield a sequence of approximating finite dimensional identification problems. We demonstrate that each of the approximating problems admits a solution and that from the resulting sequence of optimal solutions a convergent subsequence can be extracted, the limit of which is a solution to the original identification problem. The approximating identification problems can be solved using standard techniques and readily available software. Numerical results for a variety of examples are provided.

Tal-Ezer, H.: *The eigenvalues of the pseudospectral Fourier approximation to the operator $\sin(2x)\frac{\partial}{\partial x}$.* ICASE Report No. 85-8, February 7, 1985, 10 pages. Submitted to Math. Comp.

In this note we show that the eigenvalues Z_i of the pseudospectral Fourier approximation to the operator $\sin(2x)\frac{\partial}{\partial x}$ satisfy

$$R_e Z_i = \pm 1 \quad \text{or} \quad R_e Z_i = 0.$$

Whereas this does not prove stability for the Fourier method, applied to the hyperbolic equation

$$U_t = \sin(2x)U_x, \quad \pi - < x < \pi;$$

it indicates that the growth in time of the numerical solution is essentially the same as that of the solution to the differential equation.

Tal-Ezer, H.: *Spectral methods in time for parabolic problems*. ICASE Report No. 85-9, February 8, 1985, 19 pages. Submitted to SIAM J. Numer. Anal.

A pseudospectral explicit scheme for solving linear, periodic, parabolic problems is described. It has infinite accuracy both in time and in space. The high accuracy is achieved while the time resolution parameter M ($M = O(1/\Delta t)$) for time marching algorithm) and the space resolution parameter N ($N = O(1/\Delta x)$) have to satisfy $M = O(N^{1+\epsilon})$ $\epsilon > 0$, compared to the common stability condition $M = O(N^2)$ which has to be satisfied in any explicit finite order time algorithm.

Tadmor, E.: *Complex symmetric matrices with strongly stable iterates*. ICASE Report No. 85-10, February 14, 1985, 22 pages. Submitted to *Linear Algebra and Appl.*

We study complex-valued symmetric matrices. A simple expression for the spectral norm of such matrices is obtained by utilizing a unitarily congruent invariant form. Consequently, we provide a sharp criterion for identifying those symmetric matrices whose spectral norm is not exceeding one: such strongly stable matrices are usually sought in connection with convergent difference approximations to partial differential equations. As an example, we apply the derived criterion to conclude the strong stability of a Lax-Wendroff scheme.

Turkel, E.: *Algorithms for the Euler and Navier-Stokes equations for supercomputers*. ICASE Report No. 85-11, February 14, 1985, 27 pages. Proc. of "The Impact of Supercomputers in the Next Decade of CFD," Jerusalem, December 1984.

We consider the steady state Euler and Navier-Stokes equations for both compressible and incompressible flow. Methods are found for accelerating the convergence to a steady state. This acceleration is based on preconditioning the system so that it is no longer time consistent. In order that the acceleration technique be scheme independent, this preconditioning is done at the differential equation level. Applications are presented for very slow flows and also for the incompressible equations.

Pratt, T. W.: *PISCES: an environment for parallel scientific computation*. ICASE Report No. 85-12, February 15, 1985, 30 pages. Submitted to IEEE Trans. Software Engrg.

PISCES (Parallel Implementation of Scientific Computing Environments) is a project to provide high-level programming environments for parallel

MIMD computers. Pisces 1, the first of these environments, is a Fortran 77 based environment which runs under the UNIX operating system. The Pisces 1 user programs in Pisces Fortran, an extension of Fortran 77 for parallel processing. The major emphasis in the Pisces 1 design is in providing a carefully specified "virtual machine" that defines the run-time environment within which Pisces Fortran programs are executed. Each implementation then provides the same virtual machine, regardless of differences in the underlying architecture. The design is intended to be portable to a variety of architectures. Currently Pisces 1 is implemented on a network of Apollo workstations and on a DEC VAX uniprocessor via simulation of the task level parallelism. An implementation for the Flexible Computing Corp. FLEX/32 is under construction. This paper provides an introduction to the Pisces 1 virtual computer and the Fortran 77 extensions. An example of an algorithm for the iterative solution of a system of equations is given. The most notable features of the design are the provision for several different "granularities" of parallelism in programs and the provision of a "window" mechanism for distributed access to large arrays of data.

Harabetian, E.: *A convergent series expansion for hyperbolic systems of conservation laws*. ICASE Report No. 85-13, February 20, 1985, 88 pages. Submitted to Trans. Amer. Math. Soc.

We consider the discontinuous piecewise analytic initial value problem for a wide class of conservation laws that includes the full three-dimensional Euler equations. The initial interaction at an arbitrary curved surface is resolved in time by a convergent series. Among other features the solution exhibits shock, contact, and expansion waves as well as sound waves propagating on characteristic surfaces. The expansion waves correspond to the one-dimensional rarefactions but have a more complicated structure. The sound waves are generated in place of zero strength shocks, and they are caused by mismatches in derivatives.

Abarbanel, S. and D. Gottlieb: *Information content in spectral calculations*. ICASE Report No. 85-14, February 21, 1985, 13 pages. Proc. of "The Impact of Supercomputers on the Next Decade of CFD," Jerusalem, December 1984.

Spectral solutions of hyperbolic partial differential equations induce a Gibbs phenomenon near local discontinuities or strong gradients.

A procedure is presented for extracting the piecewise smooth behavior of the solution out of the oscillatory numerical solution data. The procedure is developed from the theory of linear partial differential equations. Its application to a non-linear system (the two-dimensional Euler equations of gas dynamics) is shown to be efficacious for the particular situation.

Cox, C. L. and G. J. Fix: *On the accuracy of least squares methods in the presence of corner singularities.* ICASE Report No. 85-15, February 21, 1985, 24 pages. Submitted to Math. Comp.

This paper treats elliptic problems with corner singularities. Finite element approximations based on variational principles of the least squares type tend to display poor convergence properties in such contexts. Moreover, mesh refinement or the use of special singular elements do not appreciably improve matters. Here we show that if the least squares formulation is done in appropriately weighted space, then optimal convergence results in unweighted spaces like L^2 .

Noonan, R. E. and W. R. Collins: *Construction of a menu-based system.* ICASE Report No. 85-16, February 26, 1985, 11 pages. Submitted to Software Practice and Experience.

In this paper we discuss the development of the user interface to a software code management system. The user interface was specified using a grammar and implemented using a LR parser generator. This was found to be an effective method for the rapid prototyping of a menu-based system.

Maday, Y.: *Analysis of spectral operators in one-dimensional domains.* ICASE Report No. 85-17, February 28, 1985, 26 pages. Submitted to RAIRO.

We prove results concerning certain projection operators on the space of all polynomials of degree less than or equal to N with respect to a class of one-dimensional weighted Sobolev spaces. These results are useful in the theory of the approximation of partial differential equations with spectral methods.

Roe, P. L.: *Discrete models for the numerical analysis of time-dependent multidimensional gas dynamics.* ICASE Report No. 85-18, March 1, 1985, 36 pages. Submitted to J. Comput. Phys.

This paper explores a possible technique for extending to multidimensional flows some of the upwind-differencing methods that have proved highly successful in the one-dimensional case. Attention here is concentrated on the two-dimensional case, and the flow domain is supposed to be divided into polygonal computational elements. Inside each element the flow is represented by a local superposition of elementary solutions consisting of plane waves not necessarily aligned with the element boundaries.

Zang, T. A. and M. Y. Hussaini: *A three-dimensional spectral algorithm for simulations of transition and turbulence.* ICASE Report No. 85-19, March 6, 1985, 39 pages. AIAA Paper No. 85-0296 presented at the AIAA 23rd Aerospace Sciences Meeting, January 14-17, 1985, Reno, Nevada.

A spectral algorithm for simulating three-dimensional, incompressible, parallel shear flows is described. It applies to the channel, to the parallel boundary layer, and to other shear flows with one wall-bounded and two periodic directions. Representative applications to the channel and to the heated boundary layer are presented.

Drummond, J. P., M. Y. Hussaini, and T. A. Zang: *Spectral methods for modeling supersonic chemically reacting flow fields.* ICASE Report No. 85-20, March 8, 1985, 37 pages. Submitted to AIAA J.

A numerical algorithm has been developed for solving the equations describing chemically reacting supersonic flows. The algorithm employs a two-stage Runge-Kutta method for integrating the equations in time and a Chebyshev spectral method for integrating the equations in space. The accuracy and efficiency of the technique have been assessed by comparison with an existing implicit finite-difference procedure for modeling chemically reacting flows. The comparison showed that the new procedure yielded equivalent accuracy on much coarser grids as compared to the finite-difference procedure with resultant significant gains in computational efficiency.

LeVeque, R. J: *Intermediate boundary conditions for LOD, ADI, and approximate factorization methods.* ICASE Report No. 85-21, March 17, 1985, 24 pages. Submitted to J. Comput. Phys.

A general approach to determining the correct intermediate boundary conditions for dimensional splitting methods is presented and illustrated. The intermediate solution U^* is viewed as a second-order accurate approximation to a modified equation. Deriving the modified equation and using the relationship between this equation and the original equation allows us to determine the correct boundary conditions for U^* . To illustrate this technique, we apply it to LOD and ADI methods for the heat equation in two and three space dimensions. The approximate factorization method is considered in slightly more generality.

Rosen, I. G.: *Spline-based Rayleigh-Ritz methods for the approximation of the natural modes of vibration for flexible beams with tip bodies.* ICASE Report No. 85-22, March 18, 1985, 31 pages. Submitted to Quarterly of Applied Mathematics.

Rayleigh-Ritz methods for the approximation of the natural modes for a class of vibration problems involving flexible beams with tip bodies using subspaces of piecewise polynomial spline functions are developed. An abstract operator theoretic formulation of the eigenvalue problem is derived and spectral properties investigated. The existing theory for spline-based Rayleigh-Ritz methods applied to elliptic differential operators and the approximation properties of interpolatory splines are used to argue convergence and establish rates of convergence. An example and numerical results are discussed.

Bayliss, A., L. Maestrello, P. Parikh, and E. Turkel: *Numerical simulation of boundary layer excitation by surface heating/cooling*. ICASE Report No. 85-23, March 25, 1985, 22 pages. AIAA Paper No. 85-0565, AIAA Shear Flow Control Conference, March 12-14, 1985, Boulder, CO.

This paper is a numerical study of the concept of active control of growing disturbances in an unstable compressible flow by using time periodic, localized surface heating. The simulations are calculated by a fourth-order accurate solution of the compressible, laminar Navier-Stokes equations. Fourth-order accuracy is particularly important for this problem because the solution must be computed over many wavelengths. The numerical results demonstrate the growth of an initially small fluctuation into the nonlinear regime where a local breakdown into smaller scale disturbances can be observed. It is shown that periodic surface heating over a small strip can reduce the level of the fluctuation provided that the phase of the heating current is properly chosen.

Hossain, M., G. Vahala, and D. Montgomery: *Forced MHD turbulence in a uniform external magnetic field*. ICASE Report No. 85-24, March 28, 1985, 39 pages. Submitted to Phys. Fluid.

Two-dimensional dissipative MHD turbulence is randomly driven at small spatial scales and is studied by numerical simulation in the presence of a strong uniform external magnetic field. A novel behavior is observed as being apparently distinct from the inverse cascade which prevails in the absence of an external magnetic field. The magnetic spectrum becomes dominated by the three longest-wavelength Alfvén waves in the system allowed by the boundary conditions: those which, in a box size of edge 2π have wave numbers $(k_x, k_y) = (1, 0)$, $(1, 1)$, and $(1, -1)$, where the external magnetic field is in the x direction. At any given instant, one of these three modes dominates the vector potential spectrum, but they do not constitute a resonantly coupled triad. Rather, they are apparently coupled by the smaller-scale turbulence.

ICASE COLLOQUIA

October 1, 1984 through March 31, 1985

- January 31 **Dr. Eitan Tadmor**, Tel-Aviv University: *Recovering Pointwise Values of Discontinuous Data Within Spectral Accuracy*
- February 1 **Professor J. Trevor Stuart**, Imperial College of Science and Technology: *Instability in a Squeeze Lubrication Film*
- February 8 **Mr. Pravir Dutt**, University of California, Los Angeles: *Boundary Conditions and Difference Schemes for Parabolic Systems*
- February 11 **Mr. Ke-Gang Shih**, University of Maryland: *On Axisymmetric Buckling of Nonlinearly Elastic Complete Spherical Shells*
- February 12 **Professor Kapuluru C. Reddy**, University of Tennessee Space Institute: *Spectral Approximation and Numerical Differentiation*
- February 14 **Mr. Donald French**, Cornell University: *The Finite Element Method in a Degenerate Elliptic Equation*
- February 15 **Professor Brian Cantwell**, Stanford University: *States of Motion for Jets and Vortex Rings*
- February 19 **Dr. Bertrand Mercier**, Centre D'Etudes de Limeil, France: *Resolution of Linear Hyperbolic Equations Via Methods Involving Particles*
- February 27 **Mr. Nessim Mac Giolla Mhuiris**, Cornell University: *Vortex Breakdown - A Model and Its Stability*
- February 28 **Dr. Rainald Lohner**, University College of Swansea, United Kingdom: *Finite Element Methods for Compressible Fluid Flows*

- March 7 **Professor Bradley Lucier**, Purdue University: *A Parallel Implementation of Adaptive Numerical Methods for Hyperbolic Conservation Laws*
- March 13 **Mrs. Mala Mehrotra**, The College of William and Mary: *Tree-Searching Algorithms on Parallel Architectures*
- March 18 **Ms. Valerie Miller**, University of South Carolina: *SOR Methods for Solving Large Scale Rank Deficient Least Square Problems*
- March 20 **Dr. Jittesh Gajjar**, NMI Ltd., United Kingdom: *On Some Solutions of the Navier-Stokes Equations on the ICL Distributed Array Processor*
- March 21 **Mr. Jay Albert**, Princeton University: *Monte Carlo Analysis of Ripple Transport in a Tokamak Fusion Reactor*
- March 22 **Dr. Leonhardt Kleiser**, Institute for Theoretical Fluid Mechanics, West Germany: *Numerical Simulation of Laminar-Turbulent Transition and Interactive Transition Control*
- March 22 **Professor Stanley Osher**, University of California, Los Angeles: *Uniformly High-Order Accurate Non-Oscillatory Schemes*
- March 26 **Dr. Stephen D. Brierley**, University of Minnesota: *Stability and Stabilization of Generalized Linear Systems*
- March 27 **Dr. Victor C. Dannon**, Winthrop College: *Characterizations of Entropy in Thermodynamics*
- March 28 **Professor Dan J. Inman**, State University of New York, Buffalo: *Dynamics of Non-Self-Adjoint Systems*
- March 29 **Professor Heinz-Otto Kreiss**, California Institute of Technology: *Numerical Problems Connected with Short-Range Weather Prediction*

OTHER ACTIVITIES

A Workshop on Theoretical Approaches to Turbulence hosted by ICASE/NASA was held October 10-12, 1984. The purpose of this workshop was to explore the various approaches used to study turbulence. Fourteen researchers were invited to speak and their papers will be collected into a volume published by Springer. The speakers and their topics are listed below:

- D. Bushnell, NASA Langley Research Center: *Turbulence Sensitivity and Control in Wall Flows*
- G. Chapman, NASA Ames Research Center: *Observations, Theoretical Ideas, Modelling of Turbulent Flows - Past, Present & Future*
- P. G. Saffman, California Institute of Technology: *Vortex Dynamics*
- B. B. Mandelbrot, I.B.M. Thomas J. Watson Research Center: *Fractal Geometry of Turbulence*
- J. H. Ferziger, Stanford University: *The Future of Large Eddy Simulation*
- W. D. McComb, University of Edinburgh: *Renormalisation Group Methods Applied to the Numerical Simulation of Fluid Turbulence*
- R. Herring, National Center for Atmospheric Research: *An Introduction and Overview of Various Theoretical Approaches to Turbulence*
- B. E. Launder, University of Manchester: *Progress and Prospects in Phenomenological Turbulence Models*
- M. T. Landahl, Massachusetts Institute of Technology: *Flat-Eddy Model for Coherent Structures in Boundary Layer Turbulence*
- W. C. Reynolds, Stanford University: *Impact of Large Eddy Simulation on Phenomenological Modelling of Turbulence*
- A. Pouquet, Observatoire de Nice: *Statistical Methods in Turbulence*
- D. B. Spalding, Imperial College of Science & Technology: *The Two Fluid Model of Turbulence*
- E. A. Spiegel, Columbia University: *Chaotic Dynamics in Fluids*
- R. H. Kraichnan: *Decimated Amplitude Equations for Turbulence Theory*

ICASE STAFF

October 1, 1984 through March 31, 1985

I. ADMINISTRATIVE

Milton E. Rose, Director

Ph.D., Mathematics, New York University, 1953
Numerical Methods

Robert G. Voigt, Associate Director

Ph.D., Mathematics, University of Maryland, 1969
Numerical and Computational Techniques

Linda T. Johnson, Administrative Assistant

Georgia V. Ballance, Technical Publications/Summer Housing Secretary

Etta M. Blair, Office Assistant

Personnel/Bookkeeping Secretary (Beginning December 1984)

Juanita L. Jones, Office Assistant (Beginning March 1985)

Barbara A. Kraft, Senior Technical Publications Secretary

Barbara A. Rohrbach, Personnel/Bookkeeping Secretary
Office Assistant (Through March 1985)

Emily N. Todd, Visitor Coordinator/Correspondence Secretary

II. SCIENCE COUNCIL for APPLIED MATHEMATICS and COMPUTER SCIENCE

Bruce Arden, Chairman and Arthur Doty Professor, Department of Electrical Engineering and Computer Science, Princeton University.

Andrew J. Callegari, Director, Theoretical & Mathematical Sciences Laboratory, Exxon Research & Engineering Company. (Beginning 1985)

Peter Denning, Director, RIACS, NASA/Ames Research Center. (Beginning 1985)

Michael J. Flynn, Professor, Department of Electrical Engineering, Computer Systems Laboratory, Stanford University.

Bernard Galler, Professor, Department of Computer and Communication Sciences and Associate Director of the Computer Center, University of Michigan.

C. William Gear, Professor, Department of Computer Science, University of Illinois at Urbana. (Through 1984)

Anthony C. Hearn, Department Head, Department of Information Sciences, Rand Corporation.

Herbert Keller, Professor, Physics, Math, and Astronomy, California Institute of Technology.

Seymour V. Parter, Professor, Department of Mathematics, University of Wisconsin.

Werner C. Rheinboldt, Andrew W. Mellon Professor, Department of Mathematics and Statistics, University of Pittsburgh.

Milton E. Rose, Director, Institute for Computer Applications in Science and Engineering, NASA Langley Research Center.

III. ASSOCIATE MEMBERS

Saul S. Abarbanel, Professor, Department of Applied Mathematics, Tel-Aviv University, Israel.

H. Thomas Banks, Professor, Division of Applied Mathematics, Brown University.

Peter D. Lax, Professor, Courant Institute of Mathematical Sciences, New York University.

William R. Sears, Professor, Department of Aerospace and Mechanical Engineering, University of Arizona.

IV. SENIOR STAFF SCIENTISTS

David Gottlieb - Ph.D., Numerical Analysis, Tel-Aviv University, Israel, 1972. Professor and Chairman, Department of Applied Mathematics, Tel-Aviv University. Numerical Methods for Partial Differential Equations. (July 1974 to January 1987)

M. Yousuff Hussaini - Ph.D., Mechanical Engineering, University of California, 1970. Computational Fluid Dynamics. (Beginning April 1978)

V. SCIENTIFIC STAFF

Stephen F. Davis - Ph.D., Applied Mathematics, Rensselaer Polytechnic Institute, 1980. Numerical Methods for Partial Differential Equations. (February 1982 to August 1986)

Eduard Harabetian - Ph.D., Mathematics, University of California, Los Angeles, 1984. Mathematical Analysis of Numerical Algorithms for Nonlinear Partial Differential Equations. (October 1984 to September 1985)

Murshed Hossain - Ph.D., Physics, College of William and Mary, 1983. Fluid Turbulence. (December 1983 to December 1985)

Liviu Lustman - Ph.D., Applied Mathematics, Tel-Aviv University, Israel, 1979. Numerical Methods for Partial Differential Equations, Spectral Methods, Computational Fluid Dynamics. (August 1984 to September 1986)

Vijay Naik - MS., Mechanical Engineering, University of Florida, 1982. AM., Computer Science, Duke University, 1984. Parallel Processing, Computational Fluid Dynamics. (August 1984 to August 1986)

Robert K. Powers - Ph.D., Applied Mathematics, Virginia Polytechnic Institute and State University, 1984. Numerical Techniques for Optimal Control. (March 1984 to September 1986)

Nancy E. Shoemaker - Ph.D., Mathematics, Rensselaer Polytechnic Institute, 1977. Computer Systems, particularly UNIX. (February 1982 to October 1987)

Shlomo Ta'asan - Ph.D., Applied Mathematics, Weizman Institute of Science, Israel, 1984. Multigrid Methods. (October 1984 to September 1986)

John Van Rosendale - Ph.D., Computer Science, University of Illinois, 1980. Numerical Solution of Partial Differential Equations. (June 1981 to September 1985)

VI. VISITING SCIENTISTS

Saul S. Abarbanel - Ph.D., Theoretical Aerodynamics, Massachusetts Institute of Technology, 1959. Professor, Department of Applied Mathematics, Tel-Aviv University, Israel. Numerical Analysis of Partial Differential Equations. (January to December 1985)

Dennis W. Brewer - Ph.D., Applied Mathematics, University of Wisconsin-Madison, 1975. Associate Professor, Mathematical Sciences, University of Arkansas. Control Theory. (June 1984 to August 1985)

Shahid H. Bokhari - Ph.D., Electrical and Computer Engineering, University of Massachusetts, Amherst, 1978. Associate Professor, Department of Electrical Engineering, University of Engineering and Technology, Lahore, Pakistan. Parallel Processing, Distributed Computing and Computer Architecture. (July 1984 - June 1986)

Claudio Canuto - Ph.D., Mathematics, University of Torino, Italy, 1975. Professor, Istituto de Analisi Numerica del C.N.R., Italy. Numerical Analysis. (March 1985)

Moshe Israeli - Ph.D., Applied Mathematics, Massachusetts Institute of Technology, 1971. Associate Professor, Department of Computer Science, Technion - Israel Institute of Technology. Computational Fluid Dynamics. (December 1984 - August 1985)

David A. Kopriva - Ph. D., Applied Mathematics, University of Arizona, 1982. Instructor, Department of Applied Mathematics, Massachusetts Institute of Technology. (January 1985)

Bertrand M. Mercier - Ph.D., Numerical Analysis, University of Paris, 1977. Group Leader, Department of Applied Mathematics, Centre D' Etudes De Limeil, Commissariat Al'Energie Atomique, France. (February 1985)

Robert E. Noonan - Ph.D., Computer Science, Purdue University, 1971. Professor, Department of Computer Science, College of William and Mary. Computer Systems, Multi-Processors. (September 1984 - May 1985)

Philip L. Roe - Ph.D., Cambridge University, 1962. Professor, Department of Computational Fluid Dynamics, Cranfield Institute of Technology, England. Computational Fluid Dynamics. (March 1985)

Julio Ruiz Claeysen - Ph.D., Applied Mathematics, Brown University, 1974. Professor, Department of Applied Mathematics, Universidade Federal Rio Grande do Sul, Brazil. (January - February 1985)

Eitan Tadmor - Ph.D., Numerical Analysis, Tel-Aviv University, 1979. Senior Lecturer, Department of Applied Mathematics, Tel-Aviv University, Israel. Numerical Methods for Partial Differencial Equations. (January - February 1985)

Eli Turkel - Ph.D., Applied Mathematics, New York University, 1970. Associate Professor, Department of Mathematics, Tel-Aviv University, Israel. Computational Fluid Dynamics. (January - December 1985)

Bram van Leer - Ph.D., Theoretical Astrophysic, Leiden State University, 1970. Research Leader, Department of Applied Mathematics and Computer Science, Delft University of Technology, Netherlands. Computational Fluid Dynamics. (February 1985)

VII. CONSULTANTS

Loyce M. Adams - Ph.D., Applied Mathematics, University of Virginia, 1983. Parallel Numerical Algorithms. Associate Professor, Department of Applied Mathematics, University of California, Los Angeles. Numerical Methods for Parallel Computing Systems.

Ivo Babuska - Ph.D., Technical Sciences, Tech University, Prague, Czechoslovakia, 1952; Mathematics, Academy of Sciences, Prague, 1956; D.Sc., Mathematics, Academy of Science, Prague, 1960. Professor, Institute for Physical Science and Technology, University of Maryland. Numerical Methods for Partial Differential Equations.

H. Thomas Banks - Ph.D., Applied Mathematics, Purdue University, 1967. Professor, Division of Applied Mathematics, Brown University. Control Theory and Estimation of Parameters, Mathematical Biology, Functional and Partial Differential Equations.

Alvin Bayliss - Ph.D., Mathematics, New York University, 1975. Senior Staff Scientist, Exxon Corporate Research. Numerical Methods for Partial Differential Equations.

Marsha J. Berger - Ph.D., Numerical Analysis, Stanford University, 1982. Research Associate, Courant Institute of Mathematical Sciences. Numerical Methods for Partial Differential Equations.

Achi Brandt - Ph.D. Numerical Methods, Weizman Institute of Science, Israel, 1965. Professor, The Weizman Institute, Israel. Multigrid Methods.

John A. Burns - Ph.D., Mathematics, University of Oklahoma, 1973. Professor, Virginia Polytechnic Institute and State University. Numerical Methods in Feedback Control and Parameter Estimation.

James M. Crowley - Ph.D., Applied Mathematics, Brown University, 1982. Assistant Professor, Department of Mathematics, (Captain), U.S. Air Force Academy. Identification for Distributed Parameter Systems.

Peter R. Eiseman - Ph.D., Mathematics, University of Illinois, 1970. Senior Research Scientist and Adjunct Professor, Department of Applied Physics and of Nuclear Engineering, Columbia University. Computational Fluid Dynamics.

Stefan Feyock - Ph.D., Computer Science, University of Wisconsin, 1971. Associate Professor, Department of Mathematics and Computer Science, College of William and Mary. Artificial Intelligence.

George J. Fix - Ph.D., Mathematics, Harvard University, 1968. Professor and Chairman, Department of Mathematics, Carnegie-Mellon University. Numerical Methods for Partial Differential Equations.

Joseph E. Flaherty - Ph.D., Applied Mechanics, Polytechnic Institute of Brooklyn, 1969. Professor and Chairman, Departments of Mathematical Sciences

and Computer Science, Rensselaer Polytechnic Institute. Singular Perturbations, Numerical Analysis and Applied Mathematics.

Dennis B. Gannon - Ph.D., Computer Science, University of Illinois, 1980. Assistant Professor, Department of Computer Science, Purdue University. Numerical Methods and Software and Architecture Design.

James F. Geer - Ph.D., Applied Mathematics, New York University, 1967. Professor, Systems Science and Mathematical Sciences, Watson School of Engineering, Applied Science and Technology, SUNY-Binghamton. Perturbation Methods and Asymptotic Expansions of Solutions to Partial Differential Equations.

J. Steven Gibson - Ph.D., Engineering Mechanics, University of Texas at Austin, 1975. Associate Professor, Department of Mechanical, Aerospace and Nuclear Engineering, University of California at Los Angeles. Control of Distributed Systems.

Maya Gokhale - Ph.D., Computer Science, University of Pennsylvania, 1983. Assistant Professor, Department of Computer Science, University of Delaware. Nonprocedural Languages and Parallel Processing.

Chester E. Grosch - Ph.D., Physics - Fluid Dynamics, Stevens Institute of Technology, 1967. Professor, Department of Computer Science and Slover Professor, Department of Oceanography, Old Dominion University. Hydrodynamic Stability, Computational Fluid Dynamics, Unsteady Boundary Layers and Algorithms for Array Processors.

Max D. Gunzburger - Ph.D., Mathematics, New York University, 1969. Professor, Department of Mathematics, Carnegie-Mellon University. Fluid Dynamics and Numerical Methods for Partial Differential Equations.

Subramaniya I. Hariharan - Ph.D., Mathematics, Carnegie-Mellon University, 1980. Assistant Professor, University of Tennessee Space Institute. Numerical Methods for Partial Differential Equations.

Ami Harten - Ph.D., Mathematics, Courant Institute, 1974. Associate Professor, Department of Mathematics, Tel-Aviv University, Israel. Numerical Solution for Partial Differential Equations.

Kazufumi Ito - Ph.D., Systems Science and Mathematics, Washington University, 1981. Associate Professor, Division of Applied Mathematics, Brown University. Control Theory.

Harry F. Jordan - Ph.D., Physics, University of Illinois, 1977. Professor Department of Electrical and Computer Engineering, University of Colorado at Boulder. Parallel Computation.

Ashwani K. Kapila - Ph.D., Theoretical and Applied Mechanics, Cornell University, 1975. Associate Professor, Department of Mathematical Sciences, Rensselaer Polytechnic Institute. Ordinary and Partial Differential Equations, Asymptotic Methods.

Heinz-Otto Kreiss - Ph.D., Mathematics, Royal Institute of Technology, Sweden 1960. Professor, Department of Applied Mathematics, California Institute of Technology. Numerical Analysis.

Karl K. Kunish - Ph. D., Mathematics, University of Graz, Austria. Associate Professor, Department of Mathematics, Technical University of Graz, Austria. Parameter Identification and Control.

William D. Lakin - Ph.D., Applied Mathematics, University of Chicago, 1968. Eminent Professor, Department of Mathematical Sciences, Old Dominion University. Fluid Mechanics and Elastic Vibrations.

Patricia Daniel Lamm - Ph.D., Applied Mathematics, Brown University, 1981. Assistant Professor, Department of Mathematics, Southern Methodist University. Control and Identification of Partial Differential Equations.

Robert W. MacCormack - M.S., Mathematics, Stanford University. Professor, Department of Aeronautics and Astronautics, Stanford University. Computational Fluid Dynamics and Numerical Analysis.

Piyush Mehrotra - Ph.D., Computer Science, University of Virginia, 1982. Associate Professor, Department of Computer Science, Purdue University. Programming Languages for Multiprocessor systems.

David C. Montgomery, Ph.D., Physics, Princeton, 1959. Professor, Department of Physics and Astronomy, Dartmouth College. Plasma Physics, Turbulence Theory and Magnetohydrodynamics.

Katherine A. Murphy - Ph.D., Applied Mathematics, Brown University, 1983. Visiting Assistant Professor, Department of Applied Mathematics, Brown University. Control Theory and Estimation of Parameters.

Roy A. Nicolaides - Ph.D., Mathematics, University of London, 1972. Professor, Department of Mathematics, Carnegie-Mellon University. Numerical Solution of Partial Differential Equations.

Joseph E. Oliger - Ph.D., Numerical Analysis, Uppsala University, Sweden, 1973. Associate Professor, Department of Computer Science, Stanford University. Numerical Methods for Partial Differential Equations.

James E. Ortega - Ph.D., Mathematics, Stanford University, 1962. Professor and Chairman, Department of Applied Mathematics, University of Virginia. Numerical Methods for Partial Differential Equations.

Stanley Osher - Ph.D., Functional Analysis, New York University, 1966. Professor, Department of Mathematics, University of California at Los Angeles. Methods for the Numerical Analysis of Partial Differential Equations.

Anthony Patera - Ph.D., Applied Mathematics, Massachusetts Institute of Technology, 1982. Assistant Professor, Department of Mechanical Engineering, Massachusetts Institute of Technology. Numerical Methods for Fluid Dynamics and Heat Transfer.

Merrell L. Patrick - Ph.D., Mathematics, Carnegie-Mellon University, 1964. Professor, Department of Computer Science, Duke University. Parallel Numerical Algorithms and Architectures.

Terrence W. Pratt - Ph.D., Mathematics/Computer Science, University of Texas at Austin, 1965. Professor, Department of Computer Science, University of Virginia. Programming Languages.

Daniel A. Reed - Ph.D., Computer Science, Purdue University, 1983. Assistant Professor, Department of Computer Science, University of North Carolina. Parallel Processing.

Werner C. Rheinboldt - Ph.D., Applied Mathematics, University of Freiburg, Germany, 1955. Andrew W. Mellon Professor, Department of Mathematics and Statistics, University of Pittsburgh. Numerical Analysis and Computational Solution of Nonlinear Problems.

I. Gary Rosen - Ph.D., Applied Mathematics, Brown University, 1980. Assistant Professor, Department of Applied Mathematics, University of Southern California. Numerical Methods for Problems in Control Systems.

Lawrence Sirovich - Ph.D., Fluid Mechanics, Johns Hopkins University, 1960. Professor, Division of Applied Mathematics, Brown University. Fluid Mechanics.

Edward A. Spiegel - Ph.D., Astronomy, University of Michigan, 1958. Rutherford Professor of Astronomy, Department of Astronomy and Astrophysics, University of Columbia. Mathematical Aspects of Turbulence.

Jacob T. Schwartz - Ph.D., Mathematics, Yale University, 1953. Professor, Department of Computer Science, Courant Institute for Mathematical Sciences. Programming Languages, Parallel Computing and Artificial Intelligence.

John C. Strikwerda - Ph.D., Mathematics, Stanford University, 1976. Associate Professor, Department of Computer Sciences, University of Wisconsin-Madison. Numerical Methods for Partial Differential Equations.

George M. Vahala - Ph.D., Physics, University of Iowa, 1972. Associate Professor, Department of Physics, College of William and Mary. Plasma Physics, Magnetohydrodynamics, Nonlinear Dynamics, Turbulence.

Bram van Leer - Ph.D., Theoretical Astrophysics, Leiden State University, 1970. Research Leader, Department of Applied Mathematics and Computer Science, Delft University of Technology, Netherlands. Computational Fluid Dynamics.

J. Christian Wild - Ph.D., Computer Science, Rutgers University, 1977. Assistant Professor, Department of Computer Science, Old Dominion University. Concurrent Computing Systems.

VIII. STUDENT ASSISTANTS

Mary Ann O. Bynum - Graduate student at the College of William and Mary.
(September 1984 to Present)

Eiichi Oka - Graduate student at Old Dominion University. (February 1984 to
present)

IX. GRADUATE FELLOWS

Gunilla Kreiss - Student at University of Uppsala. (March - May 1985)

Joel H. Saltz - Student at Duke University. (February - June 1985)

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